AFOSR Initiative Element: Lattice-Gas Automata and Lattice Boltzmann Methods as a Novel Parallel Computing Strategy

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Contents

Chapter 1

Executive Summary

1.1 Thrust

Phillips Laboratory has recently realized the confluence of two important events: the discovery of a spatially discreet transport theory and the construction of a cellular automata machine (CAM-8) and a wide-purpose Connection Machine-5 (CM-5). That is, there now exists first-principles lattice gas automata (LGA) and lattice Boltzmann equation (LBE) formalisms for modeling complex systems. The CAM-8 now exists as a cheap, fast parallel bit-level hardware optimized for LGA simulation. The Connection Machine-5, which has been recently installed at the Army High Performance Computing Research Center, is ideally suited to LBE simulation because of its floating-point and virtualization capabilities. Therefore, we propose a two-pronged parallel computing strategy for our thermohydrodynamic research: 1) LGA implemented on a low-cost next-generation cellular automata machine (CAM-8); and 2) LBE implemented on the Connection Machine (CM-200 and CM-5).

1.2 Approach

1.2.1 Lattice Gas Automata

LGA and LBE offer a simplified modeling strategy for handling complex and "messy" physical simulations, for example, fluids with complex interfacial boundaries throughout the entire simulation space. LGA and LBE are an efficient software tool for programming massively parallel architectures. LGA offers a unique and powerful representation of macroscopic dynamics by reducing the calculation to local space-time processes controlled within standard dynamic random access memory employing only data shifts and permutations. No central processing unit operations are required [1]. The payoff of a widely successful LGA theory, can

[1] The CAM-8 design requires no internal CPUs.

be high.

CAM is a promising platform, comparable in speed [2] and less expensive then other parallels platforms in the United States capable of running LGA calculations [3]. We will test the validly of massively fine-grained simulation and its correspondence with hydrodynamic macroscopic systems.

1.2.2 Vision

We wish to exploit LGA and LBE theory and next generation massively parallel architectures for boasting simulation rates and cost-effectiveness. Potential long-range application is: accurately model the time evolution of complex Navier-Stokes fluids.

1.3 Anticipated Benefits

1.3.1 Need of the Simulation Community

This initiative element supports the Air Force critical technology of simulation and modeling, an important new growth area for our laboratories. The Air Force objective for broad-based environmental simulations to help reduce future design and engineering costs are critically dependent on physical simulation technology. A sufficiently good physical simulation strategy and platform does not yet exist. The direction in which the Air Force simulation community is heading, although highly appealing to Air Force leaders, is actually technically very risky. Basic research in new parallel computing strategies is needed to help reduce that risk.

[2]Data shifting is handled simply by pointer manipulations.

[3]MasPar's MP-1 is a typical example with 8192 four-bit processors costing about $800K.

Chapter 2

Programmatic Description

2.1 Introduction

Request AFOSR support for a new initiative for lattice gas automata research and development of a massively parallel cellular automata machine (CAM). This research will comprise constructing a large CAM and developing hydrodynamic lattice gas automata (LGA) algorithms. This research will also comprise implementing the lattice Boltzmann equation (LBE) on state-of-the-art parallel supercomputer architectures such as the Connection Machine (CM-200 and CM-5). The hydrodynamic LGA will serve as a test-bed for demonstrating a novel parallel computing strategy which strives to capture, in the most digitally efficient and numerically stable way, accurate physical behavior of large-scale complex systems. This research will also provide for comparison of the LGA method with LBE. We will explore using a multigrid approach in connection with the lattice Boltzmann method.

2.2 Submitting Agency

Phillips Laboratory (Air Force Materiel Command), Geophysics Directorate, (PL/GPAA, Hanscom AFB, MA 01731). Manager: J. Yepez, DSN 478-2475, yepez@plh.af.mil. TAP Reference: Computational Mathematics Subarea 2304/CS, PL/GP Simulation and Applications 6670.

2.3 Lattice-Gas Automata and Lattice Boltzmann Model

LGA and LBE methods are still in a formative stage. Important engineering applications for hydrodynamic LBE currently only exist for flow through porous media. LBE is suited to parallel architectures with significant floating-point performance, high virtual-processor ratios, and efficient grid-communications. The Connection Machine is an ideal platform

for LBE. On the other hand, LGA is suited to parallel architectures optimized for fine-grained bit-level manipulations. Cellular automata machines (CAM) can be constructed inexpensively to run LGA models at unprecented rates, orders of magnitude faster than LGA models on general-purpose massively parallel computers.

A 3-D hydrodynamics model is a prototypical complex system for the LGA or LBE methodology. LGA and LBE are an efficient and physically elegant parallel programming paradigm. All calculations are local and, for LGA, can use reversible rules. Therefore the LGA and LBE programming paradigms closely mirror real-world physics which is fine-grained and time-invariant. So LGA and LBE may offer a simplified modeling strategy for handling many complex and "messy" physical simulations, i.e. cases with multiphase interfacial boundaries affect fluid flow properties. Hydrodynamics LGA and LBE may prove to be the most efficient software tool for programming massively parallel architectures.

2.4 Value to the Scientific Community

Cellular automata provide a conceptually simple and intuitive model for encoding the essential physics of complex systems. Cellular automata models of such systems offer an unique opportunity to explore a system's underlying statistical behavior. Probability distributions, correlation functions, transport properties, etc., can be explored in detail. LGA, as a discreet form of molecular dynamics simulation, provides the researcher with complete system details not obtainable by either empirical or analytical treatments. LGA as a generalization of cellular automata, offers a unique and powerful representation of macroscopic dynamics by reducing the calculation to local space-time processes, collisions and streaming, controlled within standard dynamic random access memory by employing only shifts and permutations of cell data [1]. LGA models conserve exactly, throughout the entire simulation run, all physical moments of the system, i.e. mass, energy, linear momentum, angular momentum. Consequently, LGA may prove to be a numerically stable modeling technique with performance and accuracy approaching finite-difference methods.

LBE is a generalization of LGA, where single-particle distributions are encoded directly using real numbers. The simulation dynamics is driven toward an equilibrium distribution which the modeler analytically determines a prior and encodes into the simulation algorithm. The benefit of LBE over LGA is noise reduction. However, this benefit is gained at the cost of giving up exact conservation of mass, energy, an momentum for a statistical conservation of these quantities and also at the cost of requiring expensive float-point hardware. We

[1] Update of cell data can be achieved by using fast look-up tables. In principle, no central processing unit operations are required.

understand that the actual benefit of LGA and LBE methods over more traditional methods is clearly uncertain. However, LGA and LBE merit the investment of basic research time and resources because the potential payoff of such methods, if successful, can be very large.

2.5 Anticipated Benefits to the US Air Force

Recently simulation technology has gained considerable recognition at the highest levels in the Air Force. Simulation technology is now considered a critical technology and an important new growth area for our laboratories. At Phillips Laboratory we have established the Office of Environmental Simulation. This office will help coalesce DoD resources related to environmental simulation into a state-of-the-art technology base from which system program offices, DoD engineering and research components, major defense contractors, etc., in the future may draw upon as they design new Air Force systems which are impacted by the environment–in particular, tropospheric effects. The capability to do wide ranging computer-based proof-of-concept tests of new system designs using simulation technology is hoped to be a cost effective measure leading toward reduced acquisition costs. This is perceived by Air Force leaders as an critical technology shift to stave off adverse impacts of the declining defense department budgets. Yet this direction in which the Air Force community is heading, although highly appealing to most Air Force leaders, is actually technically very risky.

Although the objective is for broad-based environmental simulations to reduce future design and engineering costs, this has in no way been proven a viable route. Currently 6.2 based simulation technology thrusts are driven by non-physical constraints. Often a model's visualization and graphics output is viewed as the critical ingredient to "good" simulation. Graphics and visualization are easily understood and consequently seem to receive high priority. Underlying physical components of such models are either missing or underemphasized and, therefore, in serious risk of large inaccuracy and numerically unstable behavior. Basic research using efficient or "quick" methods to explore certain physical properties of an environmental system will help to underprop the Air Force simulation thrust. LGA is a novel method for doing such quick physical explorations.

Most simulation technology project managers would like robust and physically based engines. But these, for the most part, do not exist because on the one hand there is the nearly overwhelming complexity of the problems and on the other hand there is the limited computational performance of desktop workstation class machines on which most current day simulation models reside.

The ambitious goals of the simulation community are not synchronized with the latest

supercomputer technology. This must be corrected for any real progress to be made in this field. The principle platform for current Air Force simulation technology is the workstation. Although the workstation's performance has reached the point where traditional mainframes are perhaps no longer as practical as they once were, workstation performance is still orders of magnitude below supercomputing levels.

The principle objective of this basic research initiative is to explore a novel parallel computing strategy which, if successful, will serve as an additional tool to aid the Air Force simulation thrust. We propose building a large fine-grained cellular automata machine (CAM), still small enough for office desk-side use, yet with a performance comparable to a massively parallel Connection Machine-200. I do not believe that such a CAM will solve the simulation grand strategy envisioned by Air Force leaders, certainly not in the near future. Nor do I believe that such a CAM will serve as general-purpose computer for engineering tasks and scientific exploration, again, certainly not in the near future. But I do believe that such a CAM is a promising platform, and being optimized for lattice gas automata (LGA) calculations, is an ideal platform for doing quick physical explorations of complex fluid systems.

The LGA approach, which can be viewed as a discreet molecular dynamics (MD) modeling approach over a discreet space and time, and the LBE approach, which can be viewed as a statistical discreet MD, are known to have application to hydrodynamics, thermohydrodynamics, magnetohydrodynamics, reaction-diffusion systems, polymer melts. In the future, it is likely, the LGA and LBE approaches should have application to geophysical problems involving fine-grained locally interacting dynamics. With this new initiative we propose building a large cellular automata machine and doing a detailed study of three-dimensional hydrodynamics including multiphase fluids. Our purpose is to see if large CAM machines can be constructed and can handle complex fluid modeling problems.

Although our hydrodynamics work may prove to be an effective tool in certain messy regimes where traditional methods are not well suited, this would be only one of the pay-offs of our new initiative research. Another pay-off will be a proof-of-concept of a novel parallel computing strategy which captures in the most digitally efficient and numerically stable way, the accurate physical behavior of complex fluid systems.

2.6 Funding

The projected total cost for the proposed basic research is supported by the Air Force Office of Scientific Research contributing core funding and new initiative funding over the five-year project cycle, fiscal year 1994 to 1998. Fiscal year 1994 funding is seed funding. The Phillips

Laboratory expenses include salaries for in-house research scientists and engineers as well as CAM design and construction costs. Out year figures for projected 6.2 and 6.3 funding level transition have not been estimated. Also not estimated are supercomputer service unit costs for the Connection Machine 200 and Connection Machine 5 at the Army High Performance Computing Research Center (AHPCRC). Resources at AHPCRC are requested under a separate but complementary proposal.

2.7 Tasks

- Develop 3-D hydrodynamic lattice gas and lattice Boltzmann automata code including multiphase fluid system. Explore lattice Boltzmann dynamics which can model a fluid system with a general equation of state.
- Test novel lattice gas computing architectures: 128 million 16-bit site CAM-8 prototype. Design 1-billion 16-bit site CAM-8-64 machine 64 modules using an SBIR vehicle.
- Explore ways of using multgrid methods in lattice Boltzmann simulations.

2.8 Schedule and Milestones

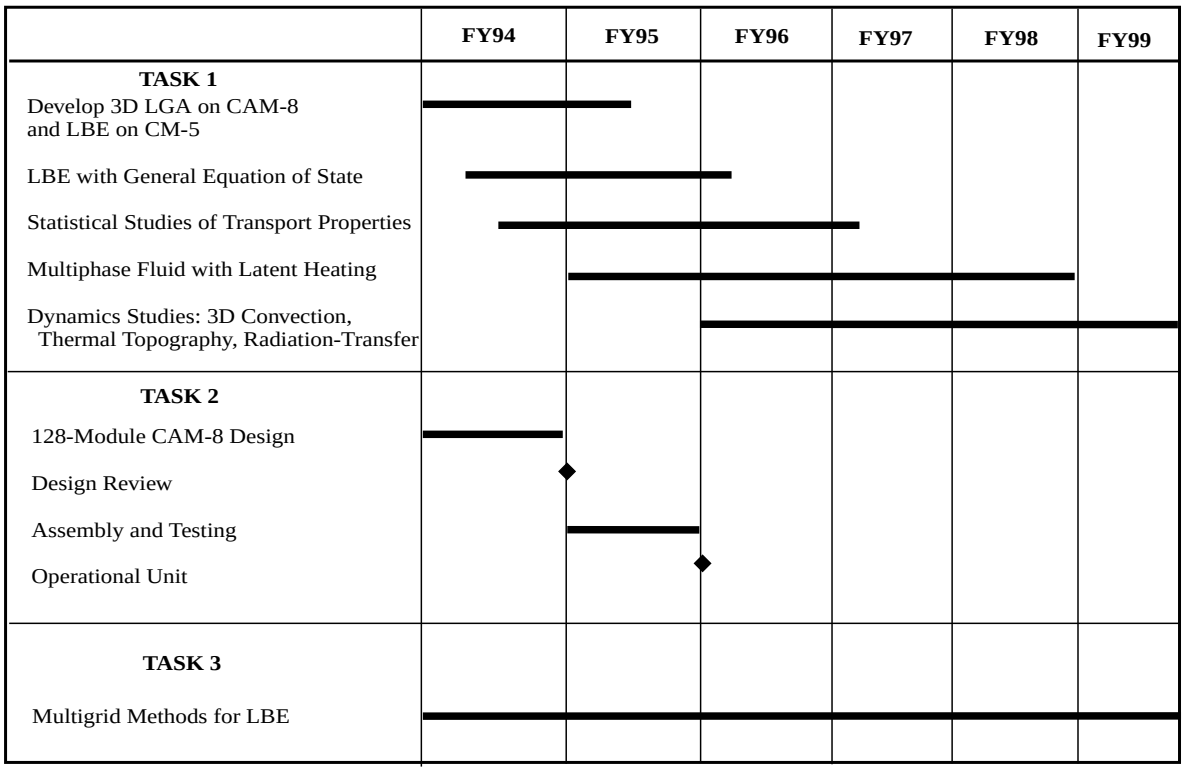

Figure 2.1: Schedule and Milestones

Chapter 3

Hydrodynamic Lattice-Gas Automata

3.1 Background

In 1983 Stephan Wolfram proposed a simple mathematical model to investigate self-organization in statistical mechanics[3]. He proposed a new "elementary" formalism which he termed cellular automata (CA) to treat dynamical systems on a discreet spatial and temporal lattice where each site or "node" of the lattice has a binary 0 or 1 value. The configuration of the discreet lattice then records the state of the dynamical field. The evolution of the field is defined by a particular set of boolean rules. Computational efficiency follows from this discrete formalism when the CA models a complex natural system with a large number of simple identical components requiring only local interaction. In this way, the CA model may be implemented on special massively parallel computers allowing one to update the state of the dynamical field at each lattice site simultaneously. This becomes computationally efficient when each site update requires knowledge of only its nearest neighbors and thereby minimizes grid communications between processors of the parallel computer. Wolfram has shown that such simple CA's possess universal features of complex nonlinear dynamical systems. Since Wolfram's seminal research, many applications of CA have been found in diverse fields including biology, chemistry, mathematics, and physics. In physics, CA's have had application in such areas as diffusion [9], hydrodynamics, information theory, magnetohydrodynamics [11], and magnetic systems [10].

Frisch et. al. have presented a CA implementation of the Navier-Stokes equation using a lattice gas automata in a two-dimensional triangular lattice [12]. In two-dimensions, for single speed automata, only on a triangular lattice does the momentum flux tensor take the correct form; and therefore, isotropy is upheld. This first lattice gas automata (LGA) simulation of two-dimensional hydrodynamic flow is call the FHP model named after its authors Frish,

Hasslacher, Pomeau. Extension of the FHP model to three-dimensions proved difficult in that momentum conservation was violated, and isotropy problems again arose. This was remedied by Dhumieres et. al. by employing a four-dimensional face-centered cubic lattice projected on to three-dimensions to implement a LGA[15]. Much numerical simulation of 2D LGA has been performed [18] and comparisons made between simulation and theory [19]. Therefore, there are well-defined prescriptions for determining fluid parameters such as Rayleigh-Taylor instability growth rates [20] and shear viscosity [21, 22, 23].

3.2 Massively Parallel Implementation

Cellular automata potentially offer a large benefit over conventional numerical techniques by their inherent computational stability and fine granularity. Yet CA's promise of being more "economical" than standard finite-difference schemes used to numerically solve partial differential equations depends upon whether or not they can be rigorously shown to emulate Navier-Stokes dynamics. Much of the work of LGA modeling has been done on two-dimensional lattices and more recently on four-dimensional lattices projected on to three-dimensions. The range of validity of the LGA implementations is still an important issue requiring further evaluation. Fundamentally, if we can validate LGA rules encoding Navier-Stokes dynamics we should expect a drastic decline in elapsed computation time as we can spread the LGA calculations over a larger and larger number of processors.

In concert with the new CA techniques, new massively parallel architectures also abound. The Connection Machine is one such platform [37] [38]. Our research in this area therefore hinges upon placing a dedicated massively parallel machine on site. Phillips Laboratory is currently evaluating candidate architectures and is conducting an informal field survey. The CM-2 and CM-5, currently at the ARMY High Performance Computing Research Center (AHPCRC) and at several universities in Massachusetts, is a convenient platform since the C-star and FORTRAN 90 parallel compilers are well advanced and ease the parallel coding workload. Machines with the Mach operating system, which is based on message passing, are also becoming available. However, despite the numerous commercial parallel computers available, the optimum platform for LGA simulations are dedicated architectures such as the CAM-8 currently development by Margolus and Toffoli at the MIT Laboratory for Computer Science [40].

Appendix A

Lattice Boltzmann Gas with a General Equation of State

A.1 Abstract

We present a simple way to add an arbitrary equation of state to a automaton gas modelled in the lattice Boltzmann limit. As a way of interpreting the lattice Boltzmann equation we present a new derivation based on an automaton Hamiltonian and the Liouville equation. A convective-gradient term added to the LBE is shown to be a sufficient route for modeling hydrodynamic flow with a general equation of state. The method generalizes to multi-speed gases in three-dimensions.

A.2 Introduction

Lattice gas methods for hydrodynamic flow over a discreet fine-grained space-time implemented on massively parallel machines like the CM-2 and CM-5 [37] or programmable matter machines like the CAM-8 [40] represent an important new avenue for practical simulations of complex physical systems. Local streaming and collision rules define a mesophysical world underlying the macroscopic system of interest. This robust computational methodology provides an exciting alternative to, and not simply an approximation of, the usual partial differential equation method of description and the associated finite difference schemes. The cellular automaton formalism, popularized in the physics community by Wolfram [4], has been extended to a more general lattice gas formalism [12, 15]. In lattice gas codes, all individual boolean bits, representing automaton particles, simultaneously propagate and rearrange within parallel architectures built from low-cost digital circuits.

Recently, this innovative lattice gas approach has been extended to the lattice Boltzmann approach [31]. In place of the detailed streaming and colliding of digital bits, one focuses

on the statistical regime where only total particle count per lattice direction per lattice node influences the dynamics, and so one neglects particle-particle correlations. Although this new approach is less noisy, it relies on expensive floating point calculations. The most practical simulation method for production work may lie somewhere between the lattice gas and lattice Boltzmann extremes. Yet the lattice Boltzmann approach offers an important analytical advantage. One may capture the essential physics of the complex system by stating no more than the system's equilibrium distribution.

Here we exploit the analytical facility of the lattice Boltzmann approach and show that the addition of a convective-gradient term in the lattice Boltzmann equation (LBE) allows one to model a hydrodynamic gaseous flow governed by a general equation of state. We restrict ourselves to single-speed automata. Thus, the system pressure may depend on local density variations. It is straightforward however to generalize our result to a multi-speed automaton gas so that the pressure dependence includes local temperature variations as well.

A.3 The Lattice Boltzmann Equation

We wish to consider a simple two-dimensional lattice Boltzmann gas defined on a discreet spatial lattice. Automaton particles stream through the lattice and undergo collisions in a similar fashion to the usual FHP model [12]. Therefore, there exists a small number of momentum states given by

$$\hat{\mathbf{e}}_\mathbf{a} = \left(\cos\frac{2\pi a}{b}, \sin\frac{2\pi a}{b}\right), \tag{A.1}$$

where $a = 1, 2, \ldots, b$. The automaton Hamiltonian is the difference of kinetic and collision terms

$$H = \frac{1}{2}\hat{\mathbf{e}}_\mathbf{a}{}^2 - \mathbf{F}\cdot\mathbf{q}. \tag{A.2}$$

Hamilton's equations for an automaton are

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}} = \hat{\mathbf{e}}_\mathbf{a} \tag{A.3}$$

and

$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}} = \mathbf{F}. \tag{A.4}$$

Liouville's equation for the distribution function may be written in terms of the automaton Hamiltonian using the Poisson bracket notation [32] as

$$\frac{\partial f_a}{\partial t} + [f_a, H] = 0 \tag{A.5}$$

where

$$[f_a, H] = \frac{\partial f_a}{\partial \mathbf{q}}\cdot\frac{\partial H}{\partial \mathbf{p}} - \frac{\partial H}{\partial \mathbf{q}}\cdot\frac{\partial f_a}{\partial \mathbf{p}}. \tag{A.6}$$

To first order and near equilibrium we may approximate a change in the distribution function by a collision as

$$\frac{\partial f_a}{\partial \mathbf{p}} = \frac{f_a - {f_a}^{eq}}{\|F\|\tau}\hat{\mathbf{F}} \tag{A.7}$$

where we have taken $\delta f_a = f_a - {f_a}^{eq}$ and introduced the collision relaxation time, τ, by writing $\delta p = \|F\|\tau$. Using Hamilton's automaton equations (A.3,A.4) and our linear approximation of $\partial f_a/\partial \mathbf{p}$ (A.7), the Poisson bracket becomes

$$[f_a, H] = \hat{\mathbf{e}}_\mathbf{a} \cdot \frac{\partial f_a}{\partial \mathbf{q}} + \frac{f_a - {f_a}^{eq}}{\tau}, \tag{A.8}$$

and so we obtain, to first order, lattice Boltzmann equation

$$\frac{\partial f_a}{\partial t} + \hat{\mathbf{e}}_\mathbf{a} \cdot \nabla f_a = -\frac{1}{\tau}(f_a - {f_a}^{eq}). \tag{A.9}$$

Shiyi Chen et. al. have arrived at (A.9) by expanding the lattice Boltzmann collision term to first order [27] about an equilibrium distribution

$$\frac{\partial f_a}{\partial t} + \hat{\mathbf{e}}_\mathbf{a} \cdot \nabla f_a = \Omega_a. \tag{A.10}$$

$$\longrightarrow \Omega_a = \Omega_a(f^{eq}) + \frac{\partial \Omega_a(f^{eq})}{\partial f_b} f_b, \tag{A.11}$$

where the zeroth-order term, $\Omega_a(f^{eq})$, must vanish by construction. The simplest ansatz for $\partial \Omega_a(f^{eq})/\partial f_b$ is to choose it to be diagonal

$$\frac{\partial \Omega_a(f^{eq})}{\partial f_b} = -\frac{1}{\tau}\delta_{ab}, \tag{A.12}$$

where again τ is the characteristic relaxation time for the simulation. Integrating (A.12) leads to the same collision term as in the R.H.S. of (A.9)

$$\Omega_a = -\frac{1}{\tau}(f_a - {f_a}^{eq}). \tag{A.13}$$

The collision term is proportional to the difference of the distribution function and its equilibrium value.

A.4 Equilibrium Distribution

To compute the system dynamics on a parallel machine we implement the exact cellular form of (A.9)

$$f_a(\mathbf{x} + \hat{\mathbf{e}}_\mathbf{a}, t+1) = f_a(\mathbf{x}, t) - \frac{1}{\tau}\left(f_a(\mathbf{x}, t) - {f_a}^{eq}(\mathbf{x}, t)\right). \tag{A.14}$$

The local cellular automaton rule (A.14) does not explicitly show any mixing of particle flow directions. That fact that (A.14) does represent collisional mixing is implicitly built into the form of ${f_a}^{eq}$ which depends on the local density and flow velocity

$$\rho = \sum_a f_a \tag{A.15}$$

and

$$\mathbf{u} = \frac{\sum_a \hat{\mathbf{e}}_\mathbf{a} f_a}{\sum_a f_a}. \tag{A.16}$$

Chen et. al. [31] have introduced a pressure-corrected lattice Boltzmann equation (PCLBE) by taking the equilibrium distribution to have the following Chapman-Enskog expansion

$${f_a}^{eq} = d + \frac{\rho D}{c^2 b}\hat{\mathbf{e}}_\mathbf{a}\cdot\mathbf{u} + \rho\frac{D(D+2)}{2c^4 b}\hat{e}_{ai}\hat{e}_{aj}u_i u_j - \frac{\rho D}{2bc^2}\mathbf{u}^2 \tag{A.17}$$

which removes the spurious effective pressure induced by the FHP flow's kinetic energy. The ideal part of the momentum flux tensor takes the correct form

$$\Pi_{ij} = \sum_a \hat{e}_{ai}\hat{e}_{aj}{f_a}^{eq} \tag{A.18}$$

$$= \frac{bd}{D}c^2\delta_{ij} + \rho u_i u_j. \tag{A.19}$$

A.5 Density Dependent Pressure

From the PCLBE in Section A.4 we know the equation of state for the isothermal gas is [31]

$$p = c_s^2\rho. \tag{A.20}$$

We now wish to consider how we may alter the LBE to allow for a more general equation of state. Let us add an additional term, h_a, to the R.H.S. of (A.9)

$$\frac{\partial f_a}{\partial t} + \hat{\mathbf{e}}_\mathbf{a}\cdot\nabla f_a = -\frac{1}{\tau}(f_a - {f_a}^{eq}) + h_a(\rho). \tag{A.21}$$

In (A.21) we have written h_a as a function of the local density. In a multi-speed model [33, 34] h_a may depend on the local temperature as well.

We wish to constrain the form of h_a so as not to violate continuity. We require

$$\sum_a h_a = 0, \tag{A.22}$$

and when $\nabla f_a = 0$,

$$\sum_a \hat{\mathbf{e}}_\mathbf{a} h_a = 0. \tag{A.23}$$

Constraint (A.23) is required only in uniform flow; i.e. for general flows $\sum_a \hat{\mathbf{e}}_\mathbf{a} h_a$ is non-zero. In the uniform flow limit the LBE reduces to

$$\frac{\partial f_a}{\partial t} = \Omega_a + h_a(\rho). \tag{A.24}$$

Summing over all lattice directions and using constraint (A.22) we have maintained the collision property that

$$\sum_a \Omega_a = 0. \tag{A.25}$$

Multiplying by $\hat{\mathbf{e}}_\mathbf{a}$, summing over directions, and using (A.23) similarly yields

$$\sum_a \hat{\mathbf{e}}_\mathbf{a} \Omega_a = 0. \tag{A.26}$$

Thus, for arbitrary flows, summing the LBE over all directions preserves continuity

$$\partial_t \sum_a f_a + \sum_a \hat{\mathbf{e}}_\mathbf{a} \cdot \nabla f_a = \sum_a \Omega_a + \sum_a h_a \tag{A.27}$$

$$\longrightarrow \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{A.28}$$

where we have used equations (A.15,A.16,A.22, and A.26).

In a similar fashion, we may arrive at Euler's equation

$$\partial_t(\rho u_i) + \partial_j(\Pi_{ij}) = \sum_a e_{ai} h_a(\rho), \tag{A.29}$$

where the momentum tensor is

$$\Pi_{ij} \equiv \sum_a e_{ai} e_{aj} f_a. \tag{A.30}$$

The R.H.S. of (A.29) imparts an effective density dependent pressure. We may expand h_a as follows

$$h_a = h_a^{(0)} + e_{aj}\partial_j h_a^{(1)} + \frac{1}{2} e_{aj} e_{ak} \partial_j \partial_k h_a^{(2)} + \frac{1}{3} e_{aj} e_{ak} e_{al} \partial_j \partial_k \partial_l h_a^{(3)} + \cdots \tag{A.31}$$

Given constraint (A.22) and the identities listed in the appendix, we immediately see that $h_a^{(0)}$ and $h_a^{(2)}$ must vanish. So the form of h_a simplifies to a total convective-gradient

$$h_a(\rho) = \hat{\mathbf{e}}_\mathbf{a} \cdot \nabla \left(\frac{D}{b} g_1(\rho) + \frac{D(D+2)}{3b} e_{ak} e_{al} \partial_k \partial_l g_2(\rho) \right), \tag{A.32}$$

where for future convenience we have introduced $g_1 = b h_a^{(1)}/D$ and $g_2 = 3b h_a^{(3)}/D(D+2)$. The R.H.S. of Euler's equation (A.29) then becomes

$$\sum_a \hat{\mathbf{e}}_\mathbf{a} h_a(\rho) = \nabla \left(g_1(\rho) + \nabla^2 g_2(\rho) \right). \tag{A.33}$$

Substituting (A.18) and (A.33) into Euler's equation (A.29) gives the Navier-Stokes equation

$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) = -\partial_i \left(c^2\rho - g_1(\rho) - \nabla^2 g_2(\rho) \right). \tag{A.34}$$

Therefore, we have arrived at an arbitrary equation state defined by functions $g_1(\rho)$ and $g_2(\rho)$. The form of the density dependent pressure follows

$$p(\rho) = c^2\rho - g_1(\rho) - \nabla^2 g_2(\rho). \tag{A.35}$$

A.6 Conclusion

We have given a new derivation of the lattice Boltzmann equation starting from a simple automaton Hamiltonian and Liouville's equations. We reviewed the LBE method and illustrated its flexibility in writing an analytical expression for the system's equilibrium distribution to remove the spurious pressure kinetic-energy dependent term characteristic of an FHP gas. Now the hydrostatic pressure correctly depends linearly on the local pressure. Given this context, we generalized the LBE by the addition of a convective-gradient term allowing us to model a hydrodynamics governed by an arbitrary equation of state.

A.7 Identities for $\hat{\mathbf{e}}_\mathbf{a}$

Our momentum states are just the complex b^{th} roots of one

$$\hat{\mathbf{e}}_\mathbf{a} = \left(\cos\frac{2\pi a}{b}, \sin\frac{2\pi a}{b} \right), \tag{A.36}$$

where $a = 1, 2, \ldots, b$. The momentum state-space has cardinality b. Lattice summations over odd powers of $\hat{\mathbf{e}}_\mathbf{a}$ must vanish by symmetry. The following identities, listed up to the fourth moment, hold for arbitrary values of b and spatial dimension D [8]

$$\sum_a e_{ai} = 0 \tag{A.37}$$

$$\sum_a e_{ai}e_{aj} = \frac{b}{D}\delta_{ij} \tag{A.38}$$

$$\sum_a e_{ai}e_{aj}e_{ak} = 0 \tag{A.39}$$

$$\sum_a e_{ai}e_{aj}e_{ak}e_{al} = \frac{b}{D(D+2)}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{A.40}$$

Bibliography

[1] T. Toffoli, Cellular automata mechanics., (Ph. D. Thesis) *Tech. Rep. No. 208*, The University of Michigan, Computer and Communication Sciences Department, 1977.

[2] T. Toffoli, Computation and construction of universality of reversible cellular automata, J. of Comp and Sys. Sci., **15**, No. 2, 213-231, 1977

[3] S. Wolfram, Statistical mechanics of cellular automata. Rev. Mod. Phys., **55**, 601-644, 1983

[4] S. Wolfram, Universality and complexity in cellular automata. Physica 10D , 1-35, 1984

[5] T. Toffoli, Cellular automata as an alternative to (rather than an approximation of) differential equations in modeling physics, Physica 10D, 117-127, 1984

[6] G.Y. Vichniac, Simulating physics with cellular automata, Physica 10D, 96-116, 1984

[7] T. Toffoli, CAM: a high-performance cellular-automaton machine, 195-204, 1984

[8] S. Wolfram, J. Stat Phys, **45**, No. 3/4, 471 (1986)

[9] B. Chopard and M. Droz, Cellular automata model for the diffusion equation. J. Stat. Phys. **64**, No. 3/4, 859-893, 1991

[10] H. Fried, The checkerboard update glauber model, cellular automata and ising-models. J. Phys. A-Math and General **23**, No. 18, 4165-4181, 1990

[11] H. Chen and W.H. Matthaeus, New cellular automaton model for magnetohydrodynamics. Phys. Rev. Letts. **58**, No. 18, 1845-1848, 1987

[12] U. Frisch, B. Hasslacher, and Y. Pomeau, Lattice-gas automata for the Navier-Stokes equation. Phys. Rev. Letts. **56**, No. 14, 1505-1508 (1986)

[13] S.A. Orszag and V. Yakhot, Reynolds number scaling of cellular-automaton hydrodynamics. Phys. Rev. Letts. **56**, No. 16, 1691-1693 (1986)

[14] N. Margolus, T. Toffoli, and G. Vichniac, Cellular-automata supercomputing for fluid-dynamics modeling. Phys. Rev. Letts. **56**, No. 16, 1694-1696 (1986)

[15] D. Dhumieres, U. Frisch, and P. Lallemand, Lattice gas models for 3D hydrodynamics. Europhys. Letts. **2**, No. 4, 291-297 (1986)

[16] U. Frish, D. d'Humieres, B. Hasslacher, P. Lallemand, Y. Pomeau, J.P. Rivet, Complex Systems, **1**, 649 (1987)

[17] C. Burges and S. Zaleski, Buoyant mixtures of cellular automaton gases. Complex Systems, **1**, 31-57 (1987)

[18] G. Zanetti, Hydrodynamics of lattice-gas automata. Phys. Rev. A **40**, No. 3, 1539-1548, 1989

[19] L.P. Kadanoff, G.R. McNamara, and G. Zanetti, From automata to fluid flow: Comparisons of simulation and theory. Phys. Rev. A **40**, No. 8, 4527-4541, 1989

[20] A.K. Gunstensen and D.H. Rothman, A lattice-gas model for three immiscible fluids, Physica D, **47**, 47-52, 1991

[21] M. Henon, Vicosity of a lattice gas, Complex Systems **1**, 739-789, 1987

[22] L.P. Kadanoff, G.R. McNamara, G. Zanetti, A poiseuille viscometer for lattice gas automata, Complex Systems **1**, 791-803, 1987

[23] J-P Rivet, Green-kubo formalism for lattice gas hydrodynamics and monte-carlo evaluation of shear viscosities, Complex Systems **1**, 839-851, 1987

[24] D.H. Rothmann, Negative-viscosity lattice gases, J. Stat. Phys, **56**, Nos. 3/4, 517-524, 1989

[25] J.P. Boon, Statistical mechanics and hydrodynamics of lattice gas automata: an overview. Physica D **47**, 3-8, 1991

[26] A.K. Gunstensen and D.H. Rothmann, A galilean-invariant immiscible lattice gas. Physica D **47**, 53-63, 1991

[27] S. Chen, G.D. Doolen, K. Eggert, D. Grunau, E.Y. Loh, Local lattice-gas model for immiscible fluids. Phys. Rev. A **43**, No. 12, 7053-7056, 1991

[28] M. Henon, Lattice-gas and lattice-boltzmann models of miscible fluids, J. Stat. Phys, **68**, Nos. 3/4, 353-377, 1992

[29] R. Holme and D.H. Rothman, Lattice-gas and lattice-boltzmann models of miscible fluids, J. Stat. Phys, **68**, Nos. 3/4, 409-429, 1992

[30] G.R. McNamara and G. Zanetti, Use of the boltzman equation to simulate lattice-gas automata, Phys Rev Lett, **61**, No. 20, 2332-2335 (1988)

[31] H. Chen, S. Chen, and W.H. Matthaeus, Recovery of the navier-stokes equations using a lattice-gas boltzmann method, Phys Rev A, **45**, No. 8, R5339 (1992)

[32] R.L. Liboff, Introduction to the theory of kinetic equations, Robert E. Krieger Publishing Co., New York, (1979)

[33] S. Chen, H. Chen, D. Martinez, and W. Matthaeus, Lattice boltzmann model for simulation of magnetohydrodynamics, Phys Rev Lett, **67**, No. 27, 3776 (1991)

[34] S. Chen, H. Chen, G.D. Doolean, S. Gutman, and M. Lee, J. Stat Phys, **62**, No. 5/6, 1121 (1991)

[35] S. Chen, Z. Wang, X. Shan, and G.D. Doolean, J. Stat Phys, **68**, No. 3/4, 379 (1992)

[36] F.J. Alexander, H. Chen, S. Chen, and G.D. Doolen, Lattice boltzmann model for compressible fluids, Phys Rev, **46**, No. 4, 1967-1970 (1992)

[37] W.D. Hillis, The connection machine. Scientific American, **256**, 108-115, 1987

[38] B.M. Boghosian, Computational physics on the connection machine. Computers in Phys., Jan/Feb, 1990

[39] P. Olsson and S.L. Johnsson, A data parallel implementation of an explicit method for the three-dimensional compressible Navier-Stokes equations. Thinking Machines Corp Tech Report, CS89-4, 1989

[40] N. Margolus and T. Toffoli, Cellular automata machines, Lattice Gas Methods for Partial Differential Equations, SFI SISOC, Eds. Doolen et al., Addison-Wesley, 219-249, 1990

[41] Despain, A., "Prospects for a lattice-gas computer," [p. 211–218]doolen.

[42] Toffoli, Tommaso, and Norman Margolus, *Cellular Automata Machines—A new environment for modeling*, MIT Press (1987). Russian translation: *Mashiny Kletochnykh Avtomatov*, Izdatelstvo "Mir" (1991), 279 pp.

[43] Clouqueur, André, and Dominique d'Humières, "RAP1, a cellular automaton machine for fluid dynamics," *Complex Systems* **1** (1987), 585–597.

[44] Smith, Mark, "Representation of geometrical and topological quantities in cellular automata," *Physica D* **45** (1990), 271–277.

[45] Margolus, Norman, "Physics and Computation" (Ph. D. Thesis) *Tech. Rep. MIT/LCS/TR-415*, MIT Laboratory for Computer Science (1988).

[46] Margolus, Norman, and Tommaso Toffoli, "Cellular automata machines," *Complex Systems* **1** (1987), 967–993; revised version in *Lattice-Gas Methods for Partial Differential Equations* (Gary Doolen et al., ed.), Addison-Wesley (1990), 219–249.